Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2017 – 03:25 am GMT

PDB ID	:	2XSZ
Title	:	The dodecameric human RuvBL1:RuvBL2 complex with truncated domains II
Authors	:	Gorynia, S.; Bandeiras, T.M.; Matias, P.M.; Pinho, F.G.; McVey, C.E.; Vonrhein, C.; Svergun, D.I.; Round, A.; Donner, P.; Carrondo, M.A.
Deposited on	:	2010-10-01
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

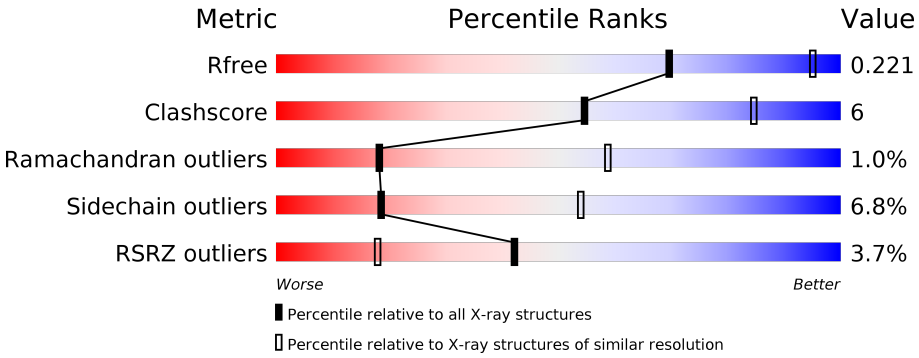
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	367	4% 70% 16% • 13%
1	B	367	5% 70% 16% • 13%
1	C	367	3% 71% 16% • 13%
2	D	378	2% 65% 16% • 18%
2	E	378	2% 62% 20% • 17%
2	F	378	2% 65% 16% • 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14664 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RUVB-LIKE 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	Se	0	0	0
			2430	1530	421	468	4	7			
1	B	319	Total	C	N	O	S	Se	0	0	0
			2435	1531	422	471	4	7			
1	C	320	Total	C	N	O	S	Se	0	0	0
			2425	1525	420	469	4	7			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	EXPRESSION TAG	UNP Q9Y265
A	2	VAL	-	EXPRESSION TAG	UNP Q9Y265
A	3	HIS	-	EXPRESSION TAG	UNP Q9Y265
A	4	HIS	-	EXPRESSION TAG	UNP Q9Y265
A	5	HIS	-	EXPRESSION TAG	UNP Q9Y265
A	6	HIS	-	EXPRESSION TAG	UNP Q9Y265
A	7	HIS	-	EXPRESSION TAG	UNP Q9Y265
A	8	HIS	-	EXPRESSION TAG	UNP Q9Y265
A	9	LEU	-	EXPRESSION TAG	UNP Q9Y265
A	10	LEU	-	EXPRESSION TAG	UNP Q9Y265
A	11	VAL	-	EXPRESSION TAG	UNP Q9Y265
A	12	PRO	-	EXPRESSION TAG	UNP Q9Y265
A	13	ARG	-	EXPRESSION TAG	UNP Q9Y265
A	14	GLY	-	EXPRESSION TAG	UNP Q9Y265
A	15	SER	-	EXPRESSION TAG	UNP Q9Y265
B	1	MSE	-	EXPRESSION TAG	UNP Q9Y265
B	2	VAL	-	EXPRESSION TAG	UNP Q9Y265
B	3	HIS	-	EXPRESSION TAG	UNP Q9Y265
B	4	HIS	-	EXPRESSION TAG	UNP Q9Y265
B	5	HIS	-	EXPRESSION TAG	UNP Q9Y265
B	6	HIS	-	EXPRESSION TAG	UNP Q9Y265
B	7	HIS	-	EXPRESSION TAG	UNP Q9Y265
B	8	HIS	-	EXPRESSION TAG	UNP Q9Y265

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	LEU	-	EXPRESSION TAG	UNP Q9Y265
B	10	LEU	-	EXPRESSION TAG	UNP Q9Y265
B	11	VAL	-	EXPRESSION TAG	UNP Q9Y265
B	12	PRO	-	EXPRESSION TAG	UNP Q9Y265
B	13	ARG	-	EXPRESSION TAG	UNP Q9Y265
B	14	GLY	-	EXPRESSION TAG	UNP Q9Y265
B	15	SER	-	EXPRESSION TAG	UNP Q9Y265
C	1	MSE	-	EXPRESSION TAG	UNP Q9Y265
C	2	VAL	-	EXPRESSION TAG	UNP Q9Y265
C	3	HIS	-	EXPRESSION TAG	UNP Q9Y265
C	4	HIS	-	EXPRESSION TAG	UNP Q9Y265
C	5	HIS	-	EXPRESSION TAG	UNP Q9Y265
C	6	HIS	-	EXPRESSION TAG	UNP Q9Y265
C	7	HIS	-	EXPRESSION TAG	UNP Q9Y265
C	8	HIS	-	EXPRESSION TAG	UNP Q9Y265
C	9	LEU	-	EXPRESSION TAG	UNP Q9Y265
C	10	LEU	-	EXPRESSION TAG	UNP Q9Y265
C	11	VAL	-	EXPRESSION TAG	UNP Q9Y265
C	12	PRO	-	EXPRESSION TAG	UNP Q9Y265
C	13	ARG	-	EXPRESSION TAG	UNP Q9Y265
C	14	GLY	-	EXPRESSION TAG	UNP Q9Y265
C	15	SER	-	EXPRESSION TAG	UNP Q9Y265

- Molecule 2 is a protein called RUVB-LIKE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	310	Total	C	N	O	S	Se	0	0	0
			2377	1487	421	457	2	10			
2	E	315	Total	C	N	O	S	Se	0	0	0
			2426	1520	428	466	2	10			
2	F	311	Total	C	N	O	S	Se	0	0	0
			2385	1493	422	458	2	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	-	EXPRESSION TAG	UNP Q9Y230
D	2	ASP	-	EXPRESSION TAG	UNP Q9Y230
D	3	TYR	-	EXPRESSION TAG	UNP Q9Y230
D	4	LYS	-	EXPRESSION TAG	UNP Q9Y230
D	5	ASP	-	EXPRESSION TAG	UNP Q9Y230
D	6	ASP	-	EXPRESSION TAG	UNP Q9Y230

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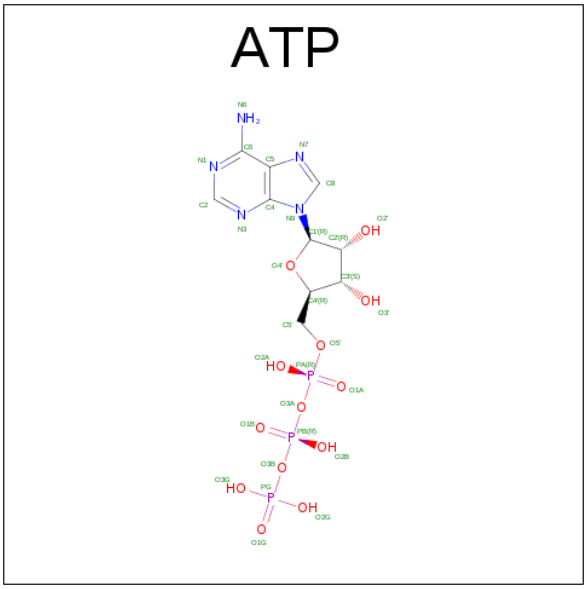
Chain	Residue	Modelled	Actual	Comment	Reference
D	7	ASP	-	EXPRESSION TAG	UNP Q9Y230
D	8	ASP	-	EXPRESSION TAG	UNP Q9Y230
D	9	LYS	-	EXPRESSION TAG	UNP Q9Y230
D	10	GLU	-	EXPRESSION TAG	UNP Q9Y230
D	11	ASN	-	EXPRESSION TAG	UNP Q9Y230
D	12	LEU	-	EXPRESSION TAG	UNP Q9Y230
D	13	TYR	-	EXPRESSION TAG	UNP Q9Y230
D	14	PHE	-	EXPRESSION TAG	UNP Q9Y230
D	15	GLN	-	EXPRESSION TAG	UNP Q9Y230
D	16	GLY	-	EXPRESSION TAG	UNP Q9Y230
E	1	MSE	-	EXPRESSION TAG	UNP Q9Y230
E	2	ASP	-	EXPRESSION TAG	UNP Q9Y230
E	3	TYR	-	EXPRESSION TAG	UNP Q9Y230
E	4	LYS	-	EXPRESSION TAG	UNP Q9Y230
E	5	ASP	-	EXPRESSION TAG	UNP Q9Y230
E	6	ASP	-	EXPRESSION TAG	UNP Q9Y230
E	7	ASP	-	EXPRESSION TAG	UNP Q9Y230
E	8	ASP	-	EXPRESSION TAG	UNP Q9Y230
E	9	LYS	-	EXPRESSION TAG	UNP Q9Y230
E	10	GLU	-	EXPRESSION TAG	UNP Q9Y230
E	11	ASN	-	EXPRESSION TAG	UNP Q9Y230
E	12	LEU	-	EXPRESSION TAG	UNP Q9Y230
E	13	TYR	-	EXPRESSION TAG	UNP Q9Y230
E	14	PHE	-	EXPRESSION TAG	UNP Q9Y230
E	15	GLN	-	EXPRESSION TAG	UNP Q9Y230
E	16	GLY	-	EXPRESSION TAG	UNP Q9Y230
F	1	MSE	-	EXPRESSION TAG	UNP Q9Y230
F	2	ASP	-	EXPRESSION TAG	UNP Q9Y230
F	3	TYR	-	EXPRESSION TAG	UNP Q9Y230
F	4	LYS	-	EXPRESSION TAG	UNP Q9Y230
F	5	ASP	-	EXPRESSION TAG	UNP Q9Y230
F	6	ASP	-	EXPRESSION TAG	UNP Q9Y230
F	7	ASP	-	EXPRESSION TAG	UNP Q9Y230
F	8	ASP	-	EXPRESSION TAG	UNP Q9Y230
F	9	LYS	-	EXPRESSION TAG	UNP Q9Y230
F	10	GLU	-	EXPRESSION TAG	UNP Q9Y230
F	11	ASN	-	EXPRESSION TAG	UNP Q9Y230
F	12	LEU	-	EXPRESSION TAG	UNP Q9Y230
F	13	TYR	-	EXPRESSION TAG	UNP Q9Y230
F	14	PHE	-	EXPRESSION TAG	UNP Q9Y230
F	15	GLN	-	EXPRESSION TAG	UNP Q9Y230
F	16	GLY	-	EXPRESSION TAG	UNP Q9Y230

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



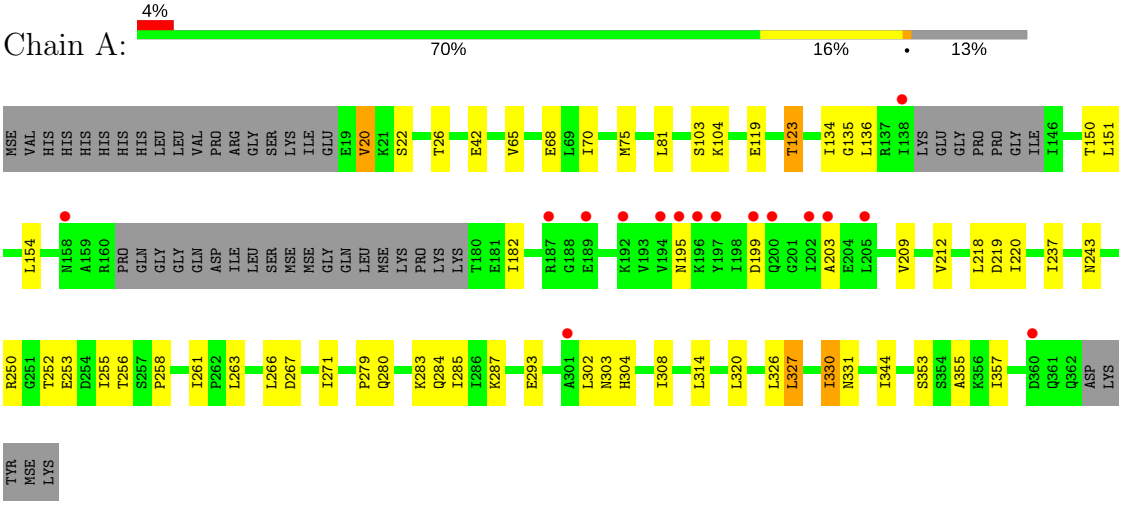
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

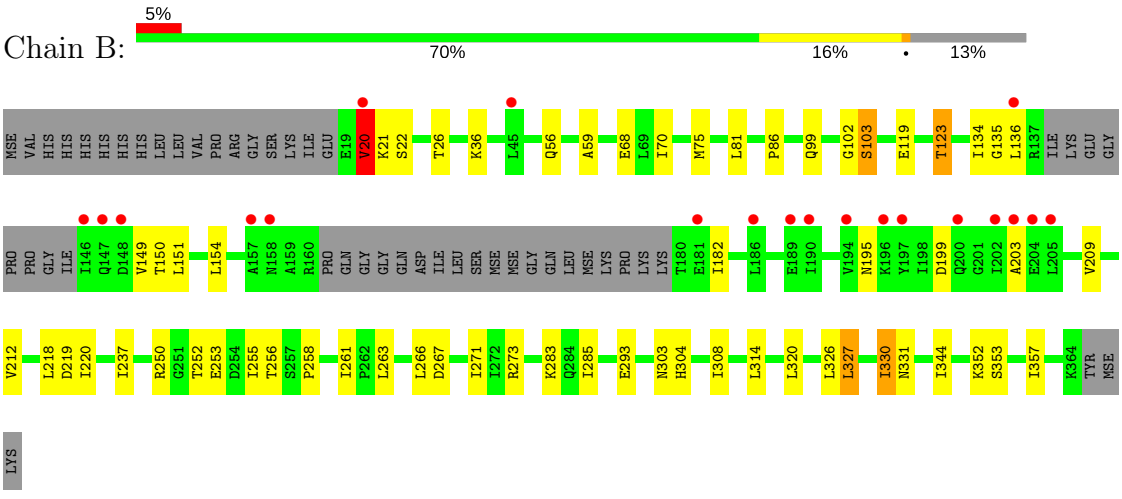
• Molecule 1: RUVB-LIKE 1

Chain A:



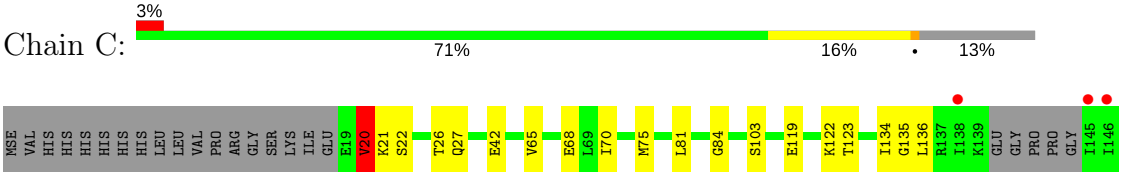
• Molecule 1: RUVB-LIKE 1

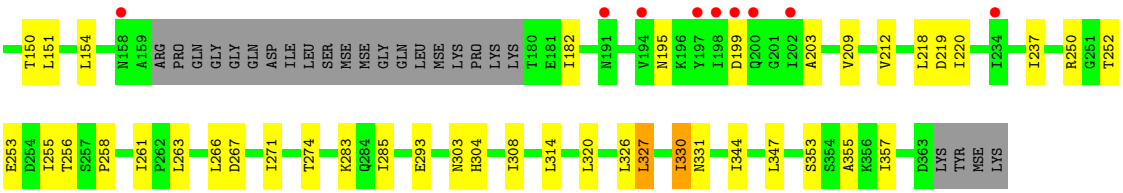
Chain B:

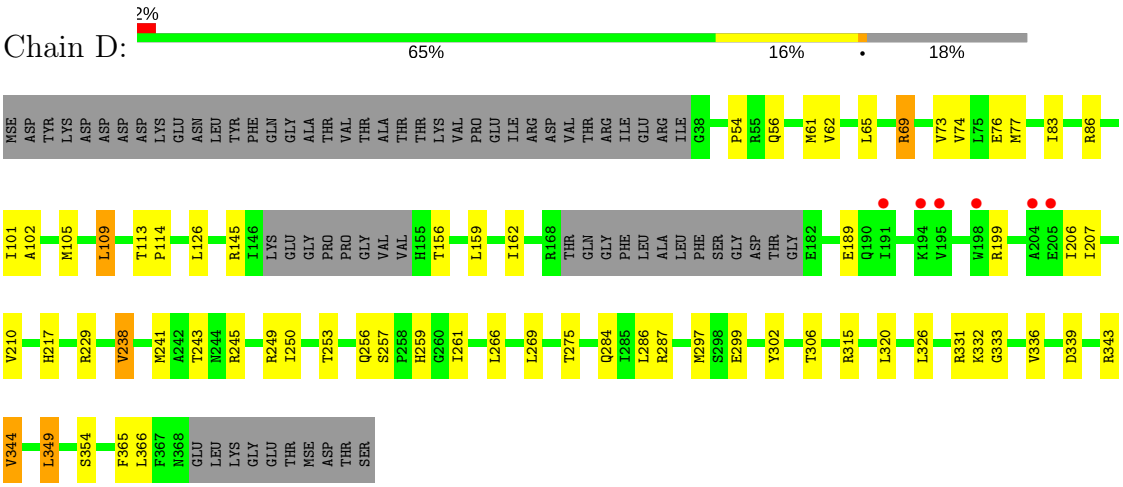


• Molecule 1: RUVB-LIKE 1

Chain C:





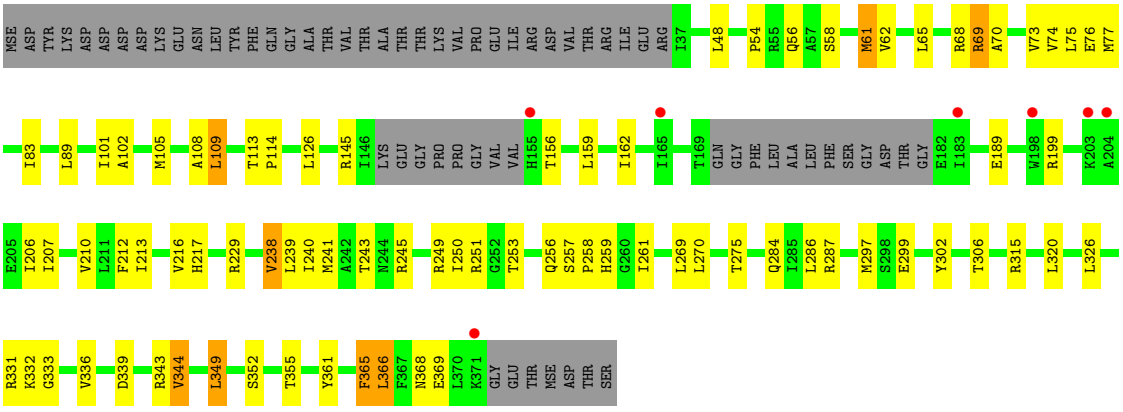


• Molecule 2: RUVB-LIKE 2

Chain D:

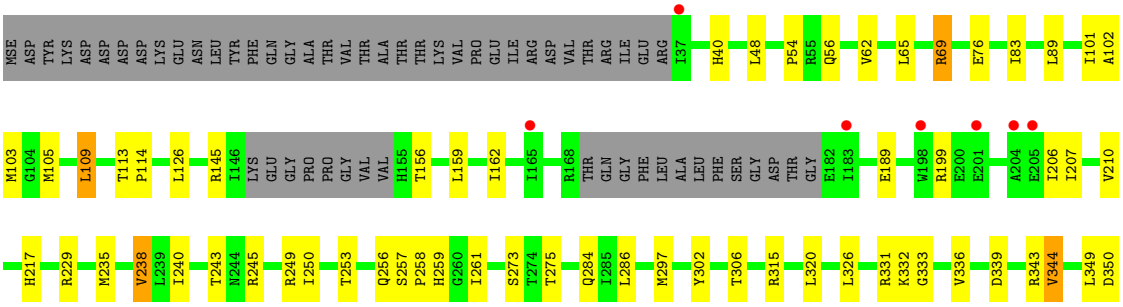
• Molecule 2: RUVB-LIKE 2

Chain E:



• Molecule 2: RUVB-LIKE 2

Chain F:




R353
F365
L366
F367
N368
GLU
LEU
LYS
GLY
GLU
THR
MSE
ASP
THR
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	111.82Å 187.93Å 244.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.14 – 3.00 46.14 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.14-3.00) 99.5 (46.14-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.0	Depositor
R, R_{free}	0.178 , 0.205 0.196 , 0.221	Depositor DCC
R_{free} test set	2628 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	85.2	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 74.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.022 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.034 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14664	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.44	0/2450	0.67	0/3294
1	B	0.44	0/2455	0.65	0/3301
1	C	0.45	0/2445	0.66	0/3289
2	D	0.45	0/2395	0.68	0/3214
2	E	0.45	0/2445	0.67	0/3280
2	F	0.47	0/2403	0.68	0/3225
All	All	0.45	0/14593	0.67	0/19603

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2430	0	2514	30	0
1	B	2435	0	2509	31	0
1	C	2425	0	2482	29	0
2	D	2377	0	2392	32	0
2	E	2426	0	2449	40	0
2	F	2385	0	2403	36	0
3	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
3	E	31	0	12	0	0
3	F	31	0	12	0	0
All	All	14664	0	14821	177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLU:HB2	2:D:326:LEU:HD21	1.53	0.88
1:B:68:GLU:HB2	2:E:326:LEU:HD21	1.55	0.85
2:E:243:THR:HG21	2:E:259:HIS:HB3	1.60	0.83
2:D:243:THR:HG21	2:D:259:HIS:HB3	1.62	0.82
2:F:243:THR:HG21	2:F:259:HIS:HB3	1.61	0.81
1:A:283:LYS:HD3	1:A:303:ASN:HA	1.66	0.76
1:C:68:GLU:HB2	2:F:326:LEU:HD21	1.71	0.73
2:F:350:ASP:OD1	2:F:353:ARG:HB2	1.91	0.70
2:E:320:LEU:HD22	2:E:344:VAL:HG13	1.76	0.67
1:B:273:ARG:HB2	2:E:349:LEU:HD11	1.77	0.65
2:E:287:ARG:NH2	2:E:299:GLU:OE1	2.30	0.65
2:E:302:TYR:O	2:E:306:THR:HG23	1.99	0.62
1:A:252:THR:HB	1:A:255:ILE:HD12	1.82	0.62
2:E:210:VAL:HG13	2:E:240:ILE:HD12	1.81	0.62
1:C:252:THR:HB	1:C:255:ILE:HD12	1.82	0.61
2:F:302:TYR:O	2:F:306:THR:HG23	2.01	0.61
1:B:252:THR:HB	1:B:255:ILE:HD12	1.81	0.61
1:C:70:ILE:HG13	1:C:75:MSE:HG3	1.83	0.61
2:D:302:TYR:O	2:D:306:THR:HG23	2.01	0.60
1:B:36:LYS:HA	1:B:99:GLN:HE21	1.66	0.60
1:C:135:GLY:HA2	1:C:150:THR:HA	1.84	0.60
2:F:286:LEU:HD12	2:F:306:THR:HG22	1.83	0.60
2:D:286:LEU:HD12	2:D:306:THR:HG22	1.84	0.60
2:D:145:ARG:HG2	2:D:156:THR:HG22	1.85	0.59
1:A:135:GLY:HA2	1:A:150:THR:HA	1.85	0.59
1:B:135:GLY:HA2	1:B:150:THR:HA	1.84	0.59
2:E:365:PHE:O	2:E:368:ASN:HB2	2.02	0.59
2:E:145:ARG:HG2	2:E:156:THR:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:145:ARG:HG2	2:F:156:THR:HG22	1.85	0.58
2:D:102:ALA:HA	2:D:105:MSE:HE3	1.86	0.57
2:E:73:VAL:HG12	2:E:77:MSE:HE2	1.87	0.57
2:F:210:VAL:HG13	2:F:240:ILE:HD12	1.85	0.57
1:B:70:ILE:HG13	1:B:75:MSE:HG3	1.86	0.56
2:D:74:VAL:HA	2:D:77:MSE:HE3	1.86	0.56
2:D:73:VAL:HG12	2:D:77:MSE:HE2	1.86	0.56
2:E:102:ALA:HA	2:E:105:MSE:HE3	1.87	0.56
2:F:102:ALA:HA	2:F:105:MSE:HE3	1.87	0.56
2:E:259:HIS:HB2	2:E:261:ILE:HD12	1.88	0.56
2:D:56:GLN:HA	2:D:65:LEU:HD21	1.87	0.56
1:A:81:LEU:HD23	1:A:271:ILE:HG12	1.88	0.56
1:A:279:PRO:O	1:A:283:LYS:HG3	2.06	0.55
2:F:56:GLN:HA	2:F:65:LEU:HD21	1.89	0.55
2:E:56:GLN:HA	2:E:65:LEU:HD21	1.89	0.54
2:D:101:ILE:HG22	2:D:105:MSE:HE2	1.88	0.54
2:D:217:HIS:CG	2:D:245:ARG:HD2	2.43	0.54
2:E:286:LEU:HD12	2:E:306:THR:HG22	1.90	0.54
2:E:101:ILE:HG22	2:E:105:MSE:HE2	1.89	0.54
2:F:217:HIS:CG	2:F:245:ARG:HD2	2.42	0.54
2:F:349:LEU:CD2	2:F:353:ARG:NH1	2.72	0.53
2:E:217:HIS:CG	2:E:245:ARG:HD2	2.43	0.53
2:F:259:HIS:HB2	2:F:261:ILE:HD12	1.89	0.53
2:D:259:HIS:HB2	2:D:261:ILE:HD12	1.91	0.53
2:F:101:ILE:HG22	2:F:105:MSE:HE2	1.91	0.53
1:C:81:LEU:HD23	1:C:271:ILE:HG12	1.91	0.52
1:A:355:ALA:HB2	2:F:258:PRO:HB3	1.91	0.52
2:D:266:LEU:HD23	2:D:269:LEU:HD12	1.92	0.52
2:E:89:LEU:HB2	2:E:269:LEU:HD13	1.91	0.52
1:B:327:LEU:HD12	1:B:344:ILE:HG12	1.90	0.52
2:E:213:ILE:HD12	2:E:239:LEU:HD11	1.91	0.52
1:A:327:LEU:HD12	1:A:344:ILE:HG12	1.92	0.52
2:F:349:LEU:HD22	2:F:353:ARG:NH1	2.25	0.52
1:A:70:ILE:HG13	1:A:75:MSE:HG3	1.91	0.51
1:A:258:PRO:HB2	1:A:266:LEU:HD21	1.93	0.51
1:B:134:ILE:HB	1:B:151:LEU:HD12	1.92	0.51
2:E:74:VAL:HG22	2:E:270:LEU:HD13	1.93	0.51
2:F:89:LEU:HD11	2:F:243:THR:HG22	1.92	0.51
1:B:209:VAL:HG22	1:B:237:ILE:HG23	1.92	0.51
1:B:81:LEU:HD23	1:B:271:ILE:HG12	1.93	0.50
1:A:209:VAL:HG22	1:A:237:ILE:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:250:ILE:HD11	2:E:257:SER:HB2	1.94	0.50
2:E:297:MSE:HG3	2:E:336:VAL:HB	1.94	0.50
2:D:297:MSE:HG3	2:D:336:VAL:HB	1.93	0.50
1:C:258:PRO:HB2	1:C:266:LEU:HD21	1.94	0.50
1:C:327:LEU:HD12	1:C:344:ILE:HG12	1.92	0.50
2:D:54:PRO:HD3	2:D:69:ARG:HB2	1.94	0.49
1:B:283:LYS:HD3	1:B:303:ASN:HA	1.94	0.49
1:A:134:ILE:HB	1:A:151:LEU:HD12	1.94	0.49
1:C:209:VAL:HG22	1:C:237:ILE:HG23	1.94	0.49
2:E:159:LEU:HA	2:E:162:ILE:HD12	1.95	0.49
2:F:249:ARG:HA	2:F:256:GLN:HA	1.95	0.49
1:A:219:ASP:HA	1:A:250:ARG:HB3	1.95	0.49
1:B:20:VAL:HG12	1:B:21:LYS:H	1.77	0.49
2:F:159:LEU:HA	2:F:162:ILE:HD12	1.95	0.49
1:C:134:ILE:HB	1:C:151:LEU:HD12	1.95	0.48
1:C:219:ASP:HA	1:C:250:ARG:HB3	1.94	0.48
2:E:212:PHE:HA	2:E:240:ILE:O	2.13	0.48
2:F:297:MSE:HG3	2:F:336:VAL:HB	1.93	0.48
2:D:159:LEU:HA	2:D:162:ILE:HD12	1.95	0.48
1:B:330:ILE:HD11	2:D:76:GLU:HG3	1.95	0.48
2:E:109:LEU:HB3	2:E:113:THR:HG21	1.95	0.48
1:B:258:PRO:HB2	1:B:266:LEU:HD21	1.94	0.48
2:D:241:MSE:HE1	2:D:269:LEU:HD21	1.96	0.48
2:E:61:MSE:HE2	2:E:68:ARG:HD2	1.94	0.48
1:B:219:ASP:HA	1:B:250:ARG:HB3	1.95	0.48
1:B:326:LEU:HD23	2:D:76:GLU:HB3	1.96	0.48
1:A:285:ILE:HG21	1:A:314:LEU:HD21	1.96	0.47
2:F:350:ASP:N	2:F:350:ASP:OD1	2.30	0.47
1:A:252:THR:O	1:A:253:GLU:HG2	2.14	0.47
2:F:250:ILE:HD11	2:F:257:SER:HB2	1.94	0.47
2:F:210:VAL:CG1	2:F:240:ILE:HD12	2.45	0.47
2:F:54:PRO:HD3	2:F:69:ARG:HB2	1.96	0.47
1:C:267:ASP:HA	2:F:315:ARG:HD2	1.95	0.47
2:E:249:ARG:HA	2:E:256:GLN:HA	1.96	0.47
1:B:267:ASP:HA	2:E:315:ARG:HD2	1.96	0.47
1:C:65:VAL:HG13	2:F:326:LEU:HD23	1.96	0.47
1:B:353:SER:O	1:B:357:ILE:HG12	2.14	0.47
2:D:250:ILE:HD11	2:D:257:SER:HB2	1.95	0.47
2:D:349:LEU:HD12	2:D:354:SER:HA	1.97	0.47
1:A:320:LEU:HD22	1:A:344:ILE:HG22	1.97	0.46
1:A:353:SER:O	1:A:357:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:GLY:HA3	1:C:274:THR:OG1	2.15	0.46
2:D:109:LEU:HB3	2:D:113:THR:HG21	1.96	0.46
1:A:123:THR:HG23	2:D:126:LEU:HB3	1.98	0.46
2:D:249:ARG:HA	2:D:256:GLN:HA	1.96	0.46
1:B:252:THR:O	1:B:253:GLU:HG2	2.15	0.46
2:E:216:VAL:HG21	2:E:241:MSE:SE	2.66	0.46
1:C:353:SER:O	1:C:357:ILE:HG12	2.16	0.45
1:C:320:LEU:HD22	1:C:344:ILE:HG22	1.98	0.45
1:B:320:LEU:HD22	1:B:344:ILE:HG22	1.98	0.45
1:C:212:VAL:HG11	1:C:218:LEU:HD11	1.99	0.45
1:C:326:LEU:HD23	2:E:76:GLU:HB3	1.99	0.45
1:A:330:ILE:HG22	1:A:331:ASN:HD22	1.82	0.45
1:C:252:THR:O	1:C:253:GLU:HG2	2.17	0.45
1:C:330:ILE:HG22	1:C:331:ASN:HD22	1.82	0.45
1:C:283:LYS:HD3	1:C:303:ASN:HA	1.98	0.45
2:E:366:LEU:O	2:E:369:GLU:HB2	2.16	0.45
2:E:54:PRO:HD3	2:E:69:ARG:HB2	2.00	0.44
1:C:20:VAL:HG12	1:C:21:LYS:H	1.83	0.44
1:B:330:ILE:HG22	1:B:331:ASN:HD22	1.83	0.44
1:C:122:LYS:HD2	2:F:126:LEU:HD21	2.00	0.43
1:B:123:THR:HG23	2:E:126:LEU:HB3	2.01	0.43
1:A:287:LYS:HB2	1:A:302:LEU:HD21	1.99	0.43
1:A:330:ILE:HD11	2:F:76:GLU:HG3	1.99	0.43
2:F:109:LEU:HB3	2:F:113:THR:HG21	1.99	0.43
1:A:151:LEU:HA	1:A:154:LEU:HD12	1.99	0.43
1:B:136:LEU:HD22	1:B:203:ALA:HB1	2.01	0.43
1:B:261:ILE:HB	1:B:266:LEU:HD13	2.01	0.43
1:C:151:LEU:HA	1:C:154:LEU:HD12	2.01	0.43
2:F:320:LEU:HD22	2:F:344:VAL:HG13	2.00	0.43
1:A:261:ILE:HB	1:A:266:LEU:HD13	2.01	0.43
2:F:114:PRO:HD3	2:F:207:ILE:HD12	2.01	0.43
2:D:114:PRO:HD3	2:D:207:ILE:HD12	2.01	0.43
1:B:151:LEU:HA	1:B:154:LEU:HD12	2.00	0.42
1:B:212:VAL:HG11	1:B:218:LEU:HD11	2.01	0.42
1:B:304:HIS:O	1:B:308:ILE:HG12	2.19	0.42
2:E:114:PRO:HD3	2:E:207:ILE:HD12	2.02	0.42
1:A:136:LEU:HD22	1:A:203:ALA:HB1	2.01	0.42
1:A:65:VAL:HG13	2:D:326:LEU:HD23	2.00	0.42
2:F:349:LEU:HD22	2:F:353:ARG:CZ	2.49	0.42
1:B:285:ILE:HG21	1:B:314:LEU:HD21	2.00	0.42
2:E:210:VAL:HG22	2:E:238:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASP:HA	2:D:315:ARG:HD2	2.02	0.42
2:E:62:VAL:HG21	2:E:284:GLN:HB3	2.02	0.42
1:B:56:GLN:HG3	1:B:59:ALA:HB3	2.02	0.42
1:C:304:HIS:O	1:C:308:ILE:HG12	2.20	0.42
1:B:86:PRO:HD2	2:E:361:TYR:OH	2.20	0.42
2:E:75:LEU:HD21	2:E:108:ALA:HB3	2.02	0.42
1:A:212:VAL:HG11	1:A:218:LEU:HD11	2.01	0.41
2:D:284:GLN:HE22	2:D:287:ARG:HD2	1.85	0.41
1:C:285:ILE:HG21	1:C:314:LEU:HD21	2.02	0.41
1:C:136:LEU:HD22	1:C:203:ALA:HB1	2.02	0.41
1:C:355:ALA:HB2	2:E:258:PRO:HB3	2.01	0.41
2:D:320:LEU:HD22	2:D:344:VAL:HG13	2.02	0.41
2:D:62:VAL:HG21	2:D:284:GLN:HB3	2.03	0.41
1:A:326:LEU:HD23	2:F:76:GLU:HB3	2.02	0.41
1:C:347:LEU:HB3	2:E:70:ALA:HB2	2.03	0.41
2:D:287:ARG:NH2	2:D:299:GLU:OE1	2.54	0.41
2:F:210:VAL:HG22	2:F:238:VAL:HG13	2.02	0.41
2:F:62:VAL:HG21	2:F:284:GLN:HB3	2.02	0.41
1:A:280:GLN:HE21	1:A:284:GLN:HG3	1.86	0.41
1:C:261:ILE:HB	1:C:266:LEU:HD13	2.02	0.41
1:B:20:VAL:HG13	1:B:149:VAL:HG13	2.03	0.40
1:A:304:HIS:O	1:A:308:ILE:HG12	2.21	0.40
2:E:284:GLN:HE22	2:E:287:ARG:HD2	1.87	0.40
2:F:297:MSE:HE2	2:F:302:TYR:HA	2.03	0.40
2:F:40:HIS:HB2	2:F:103:MSE:HE3	2.04	0.40
2:D:210:VAL:HG22	2:D:238:VAL:HG13	2.01	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/367 (85%)	296 (95%)	12 (4%)	4 (1%)	14	51
1	B	313/367 (85%)	296 (95%)	12 (4%)	5 (2%)	11	46
1	C	314/367 (86%)	299 (95%)	12 (4%)	3 (1%)	18	59
2	D	304/378 (80%)	295 (97%)	7 (2%)	2 (1%)	25	67
2	E	309/378 (82%)	300 (97%)	7 (2%)	2 (1%)	28	70
2	F	305/378 (81%)	297 (97%)	6 (2%)	2 (1%)	25	67
All	All	1857/2235 (83%)	1783 (96%)	56 (3%)	18 (1%)	18	59

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	104	LYS
1	B	20	VAL
1	C	20	VAL
2	D	332	LYS
2	E	332	LYS
2	F	332	LYS
1	B	103	SER
2	F	333	GLY
1	A	22	SER
1	B	22	SER
1	B	102	GLY
1	C	22	SER
2	D	333	GLY
2	E	333	GLY
1	A	182	ILE
1	C	182	ILE
1	B	182	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/299 (89%)	252 (94%)	15 (6%)	25	62
1	B	267/299 (89%)	253 (95%)	14 (5%)	27	65
1	C	263/299 (88%)	248 (94%)	15 (6%)	24	62
2	D	250/305 (82%)	231 (92%)	19 (8%)	15	48
2	E	257/305 (84%)	234 (91%)	23 (9%)	11	40
2	F	251/305 (82%)	232 (92%)	19 (8%)	15	48
All	All	1555/1812 (86%)	1450 (93%)	105 (7%)	18	54

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	26	THR
1	A	42	GLU
1	A	103	SER
1	A	119	GLU
1	A	123	THR
1	A	195	ASN
1	A	199	ASP
1	A	220	ILE
1	A	243	ASN
1	A	256	THR
1	A	263	LEU
1	A	293	GLU
1	A	327	LEU
1	A	330	ILE
1	B	20	VAL
1	B	26	THR
1	B	103	SER
1	B	119	GLU
1	B	123	THR
1	B	195	ASN
1	B	199	ASP
1	B	220	ILE
1	B	256	THR
1	B	263	LEU
1	B	293	GLU
1	B	327	LEU

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Mol	Chain	Res	Type
1	B	330	ILE
1	B	352	LYS
1	C	20	VAL
1	C	26	THR
1	C	27	GLN
1	C	42	GLU
1	C	103	SER
1	C	119	GLU
1	C	123	THR
1	C	195	ASN
1	C	199	ASP
1	C	220	ILE
1	C	256	THR
1	C	263	LEU
1	C	293	GLU
1	C	327	LEU
1	C	330	ILE
2	D	61	MSE
2	D	69	ARG
2	D	83	ILE
2	D	86	ARG
2	D	109	LEU
2	D	189	GLU
2	D	199	ARG
2	D	206	ILE
2	D	229	ARG
2	D	238	VAL
2	D	253	THR
2	D	275	THR
2	D	331	ARG
2	D	339	ASP
2	D	343	ARG
2	D	344	VAL
2	D	349	LEU
2	D	365	PHE
2	D	366	LEU
2	E	48	LEU
2	E	58	SER
2	E	61	MSE
2	E	69	ARG
2	E	83	ILE
2	E	109	LEU

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Mol	Chain	Res	Type
2	E	189	GLU
2	E	199	ARG
2	E	206	ILE
2	E	229	ARG
2	E	238	VAL
2	E	251	ARG
2	E	253	THR
2	E	275	THR
2	E	331	ARG
2	E	339	ASP
2	E	343	ARG
2	E	344	VAL
2	E	349	LEU
2	E	352	SER
2	E	355	THR
2	E	365	PHE
2	E	366	LEU
2	F	48	LEU
2	F	69	ARG
2	F	83	ILE
2	F	109	LEU
2	F	189	GLU
2	F	199	ARG
2	F	206	ILE
2	F	229	ARG
2	F	235	MSE
2	F	238	VAL
2	F	253	THR
2	F	273	SER
2	F	275	THR
2	F	331	ARG
2	F	339	ASP
2	F	343	ARG
2	F	344	VAL
2	F	365	PHE
2	F	366	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	280	GLN

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Mol	Chain	Res	Type
1	A	284	GLN
1	A	331	ASN
1	B	48	GLN
1	B	99	GLN
1	B	284	GLN
1	B	331	ASN
1	C	48	GLN
1	C	58	ASN
1	C	284	GLN
1	C	331	ASN
2	D	217	HIS
2	D	284	GLN
2	D	337	GLN
2	D	362	GLN
2	E	217	HIS
2	E	284	GLN
2	E	362	GLN
2	F	217	HIS
2	F	284	GLN
2	F	337	GLN
2	F	362	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	A	501	-	27,33,33	1.91	5 (18%)	25,52,52	0.79	0
3	ATP	B	501	-	27,33,33	1.76	6 (22%)	25,52,52	0.97	1 (4%)
3	ATP	C	501	-	27,33,33	1.69	4 (14%)	25,52,52	0.99	1 (4%)
3	ATP	D	501	-	27,33,33	1.36	4 (14%)	25,52,52	0.80	1 (4%)
3	ATP	E	501	-	27,33,33	1.43	5 (18%)	25,52,52	0.74	0
3	ATP	F	501	-	27,33,33	1.33	7 (25%)	25,52,52	0.89	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	501	-	-	0/18/38/38	0/3/3/3
3	ATP	B	501	-	-	0/18/38/38	0/3/3/3
3	ATP	C	501	-	-	0/18/38/38	0/3/3/3
3	ATP	D	501	-	-	0/18/38/38	0/3/3/3
3	ATP	E	501	-	-	0/18/38/38	0/3/3/3
3	ATP	F	501	-	-	0/18/38/38	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	ATP	C8-N7	-2.56	1.29	1.34
3	E	501	ATP	C8-N7	-2.47	1.30	1.34
3	B	501	ATP	C8-N7	-2.42	1.30	1.34
3	F	501	ATP	C8-N7	-2.25	1.30	1.34
3	D	501	ATP	PG-O3B	2.09	1.63	1.60
3	F	501	ATP	C2-N3	2.18	1.35	1.32
3	E	501	ATP	PG-O1G	2.18	1.58	1.50
3	F	501	ATP	C4-N3	2.21	1.38	1.35
3	F	501	ATP	PG-O1G	2.23	1.58	1.50
3	B	501	ATP	C2-N1	2.25	1.38	1.33
3	E	501	ATP	C2-N1	2.26	1.38	1.33
3	D	501	ATP	C2-N1	2.38	1.38	1.33
3	F	501	ATP	O4'-C1'	2.38	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	ATP	PG-O1G	2.38	1.58	1.50
3	C	501	ATP	PG-O1G	2.43	1.59	1.50
3	F	501	ATP	C2-N1	2.45	1.38	1.33
3	A	501	ATP	PG-O1G	2.47	1.59	1.50
3	F	501	ATP	PG-O3B	2.51	1.64	1.60
3	C	501	ATP	C2-N3	2.84	1.36	1.32
3	D	501	ATP	C2-N3	3.10	1.37	1.32
3	E	501	ATP	C2-N3	3.38	1.37	1.32
3	E	501	ATP	O4'-C1'	3.49	1.46	1.41
3	A	501	ATP	C2-N3	3.61	1.38	1.32
3	B	501	ATP	C2-N3	3.67	1.38	1.32
3	D	501	ATP	O4'-C1'	3.97	1.46	1.41
3	B	501	ATP	O4'-C1'	4.12	1.47	1.41
3	C	501	ATP	O4'-C1'	4.36	1.47	1.41
3	B	501	ATP	PG-O3B	4.89	1.68	1.60
3	C	501	ATP	PG-O3B	4.95	1.68	1.60
3	A	501	ATP	O4'-C1'	5.12	1.48	1.41
3	A	501	ATP	PG-O3B	5.58	1.69	1.60

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	ATP	N3-C2-N1	-2.88	126.35	128.86
3	B	501	ATP	N3-C2-N1	-2.61	126.58	128.86
3	F	501	ATP	N3-C2-N1	-2.08	127.05	128.86
3	D	501	ATP	C5-C6-N6	2.04	124.63	120.47
3	F	501	ATP	C5-C6-N6	2.19	124.94	120.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	311/367 (84%)	0.03	16 (5%)	29	12	69, 97, 173, 214	1 (0%)
1	B	312/367 (85%)	0.16	20 (6%)	20	7	74, 113, 169, 211	1 (0%)
1	C	313/367 (85%)	0.06	12 (3%)	41	17	71, 104, 170, 205	1 (0%)
2	D	300/378 (79%)	-0.02	6 (2%)	65	36	74, 106, 168, 202	0
2	E	305/378 (80%)	-0.08	7 (2%)	61	31	79, 108, 167, 196	0
2	F	301/378 (79%)	0.01	7 (2%)	61	31	66, 97, 160, 188	0
All	All	1842/2235 (82%)	0.03	68 (3%)	42	18	66, 105, 169, 214	3 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	146	ILE	4.7
1	B	189	GLU	4.7
1	A	194	VAL	4.2
1	B	147	GLN	4.2
1	A	202	ILE	4.1
1	C	202	ILE	4.0
1	C	191	ASN	3.8
1	A	192	LYS	3.8
2	F	165	ILE	3.7
1	B	148	ASP	3.7
1	A	200	GLN	3.6
2	F	205	GLU	3.6
1	B	202	ILE	3.6
1	B	194	VAL	3.5
2	D	198	TRP	3.5
1	B	146	ILE	3.4
1	C	145	ILE	3.3
1	A	203	ALA	3.3
1	B	197	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	197	TYR	3.2
1	B	136	LEU	3.2
1	B	186	LEU	3.2
1	C	194	VAL	3.1
1	B	190	ILE	3.1
1	A	138	ILE	3.0
2	F	37	ILE	3.0
1	A	199	ASP	3.0
2	E	371	LYS	3.0
1	B	158	ASN	3.0
2	E	155	HIS	3.0
1	A	189	GLU	2.9
1	B	203	ALA	2.8
2	E	198	TRP	2.8
1	C	234	ILE	2.8
1	A	195	ASN	2.8
2	F	183	ILE	2.8
2	F	198	TRP	2.7
1	C	199	ASP	2.7
1	C	198	ILE	2.6
1	B	204	GLU	2.6
2	D	191	ILE	2.6
2	E	165	ILE	2.6
1	A	360	ASP	2.5
2	D	205	GLU	2.5
1	B	205	LEU	2.4
2	E	203	LYS	2.4
1	C	158	ASN	2.4
1	B	157	ALA	2.4
1	A	196	LYS	2.4
2	E	183	ILE	2.4
2	D	194	LYS	2.4
1	B	200	GLN	2.3
1	A	187	ARG	2.3
1	A	205	LEU	2.3
2	D	195	VAL	2.2
1	B	45	LEU	2.2
1	C	138	ILE	2.2
2	F	201	GLU	2.2
2	E	204	ALA	2.1
1	C	200	GLN	2.1
1	A	158	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	196	LYS	2.1
1	B	20	VAL	2.1
1	A	301	ALA	2.1
2	D	204	ALA	2.0
1	B	181	GLU	2.0
2	F	204	ALA	2.0
1	A	197	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ATP	E	501	31/31	0.92	0.21	0.52	87,92,124,126	0
3	ATP	B	501	31/31	0.85	0.28	0.23	93,97,133,134	0
3	ATP	C	501	31/31	0.93	0.23	0.17	83,88,134,134	0
3	ATP	F	501	31/31	0.93	0.20	-0.04	77,84,117,119	0
3	ATP	A	501	31/31	0.93	0.20	-0.28	77,81,123,124	0
3	ATP	D	501	31/31	0.91	0.20	-0.49	90,96,120,121	0

6.5 Other polymers (i)

There are no such residues in this entry.